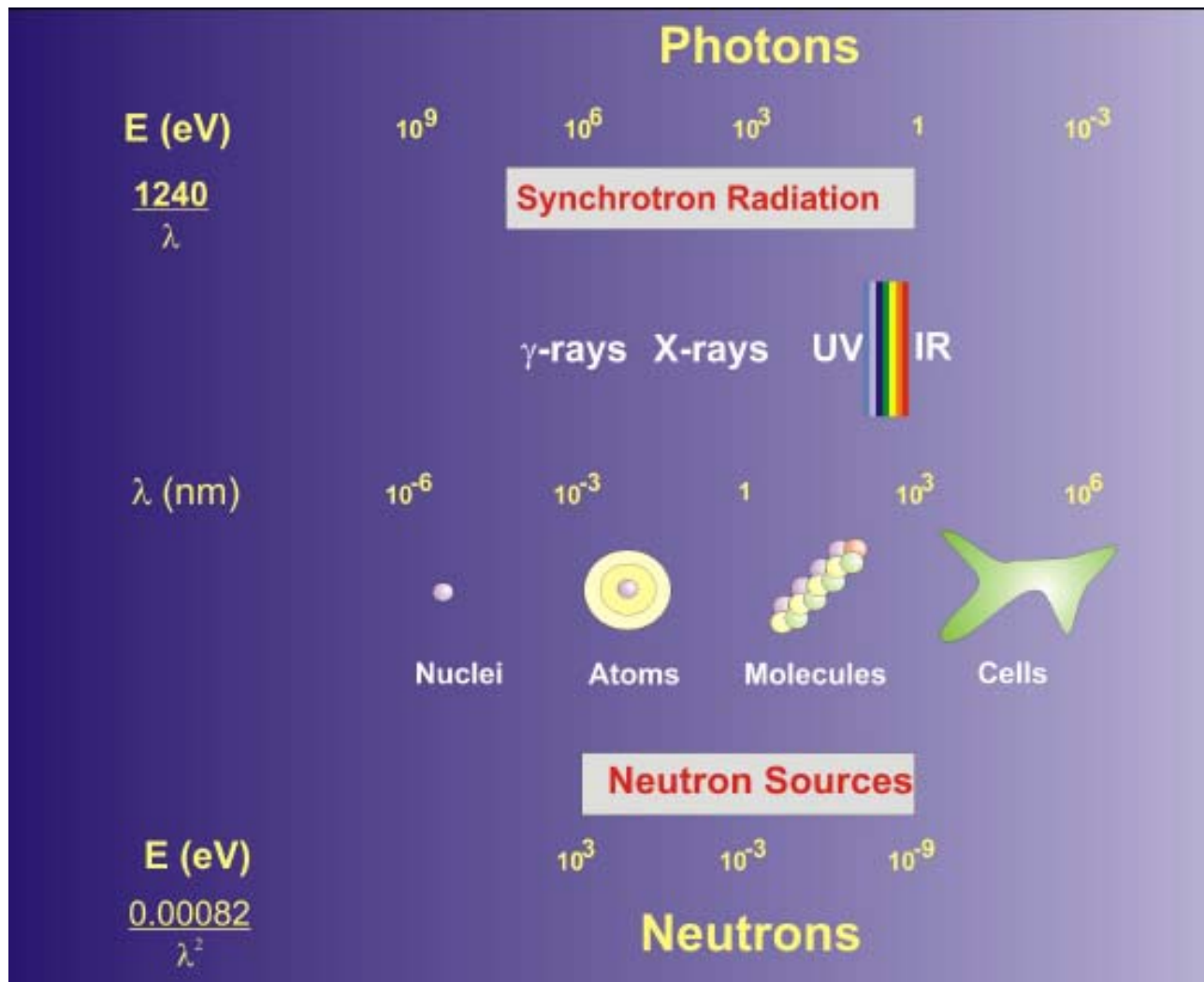


Tenth National School on Neutron and X-ray Scattering



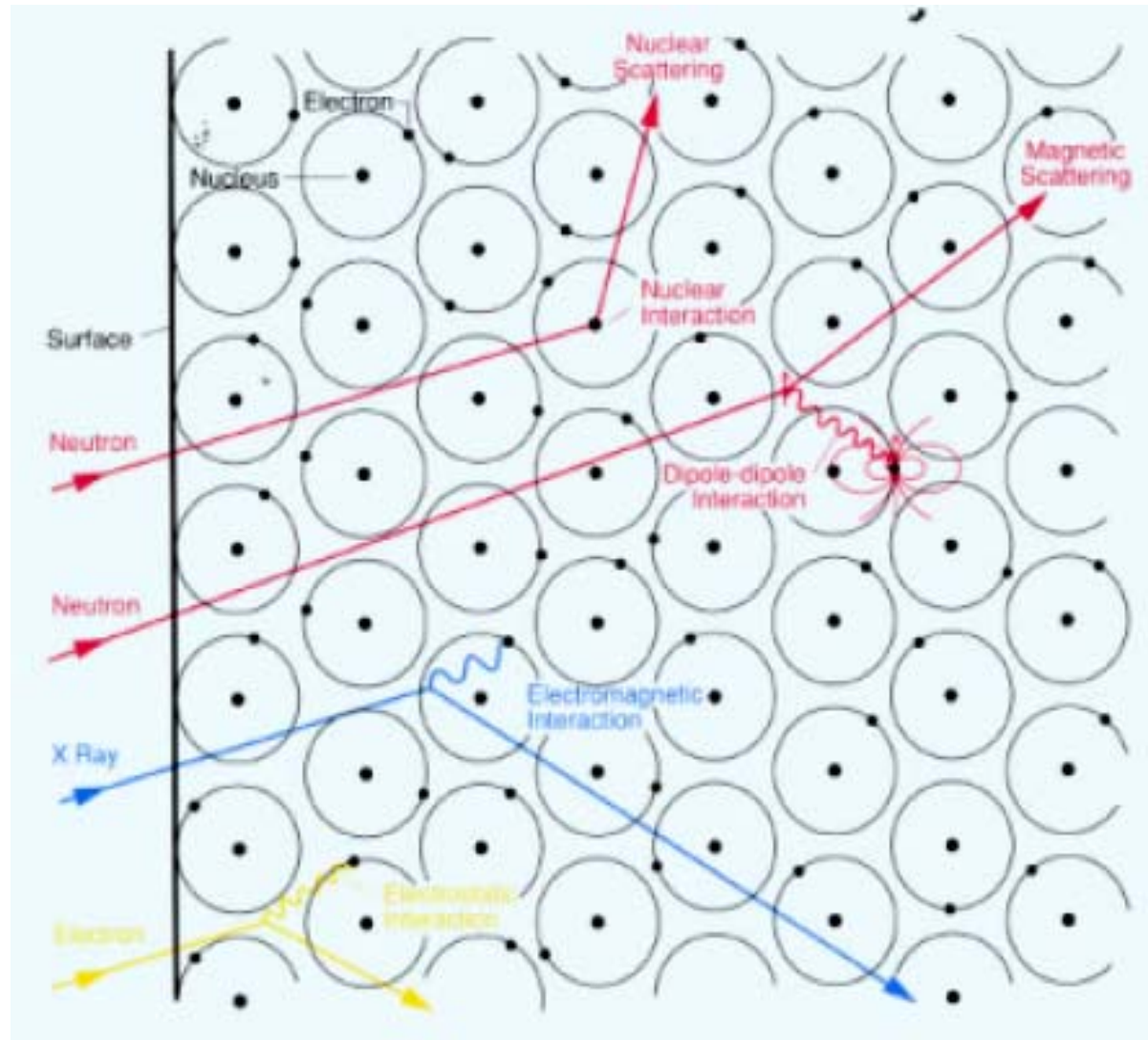
Why Neutron and X-ray?



X-ray
 $0.1-10 \text{ \AA}$
 $1-100 \text{ keV}$

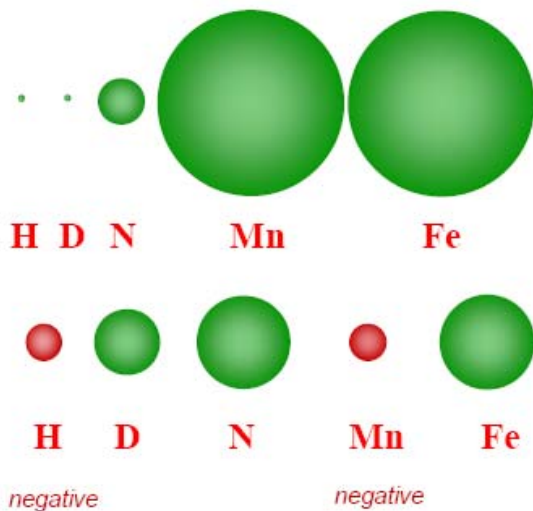
Neutron
 $0.3-3 \text{ \AA}$
 $0.1-1000 \text{ meV}$

Interaction of Neutron and X-ray with Matter



Neutron vs. X-ray

X-ray scattering length



- **Synchrotron X-rays**

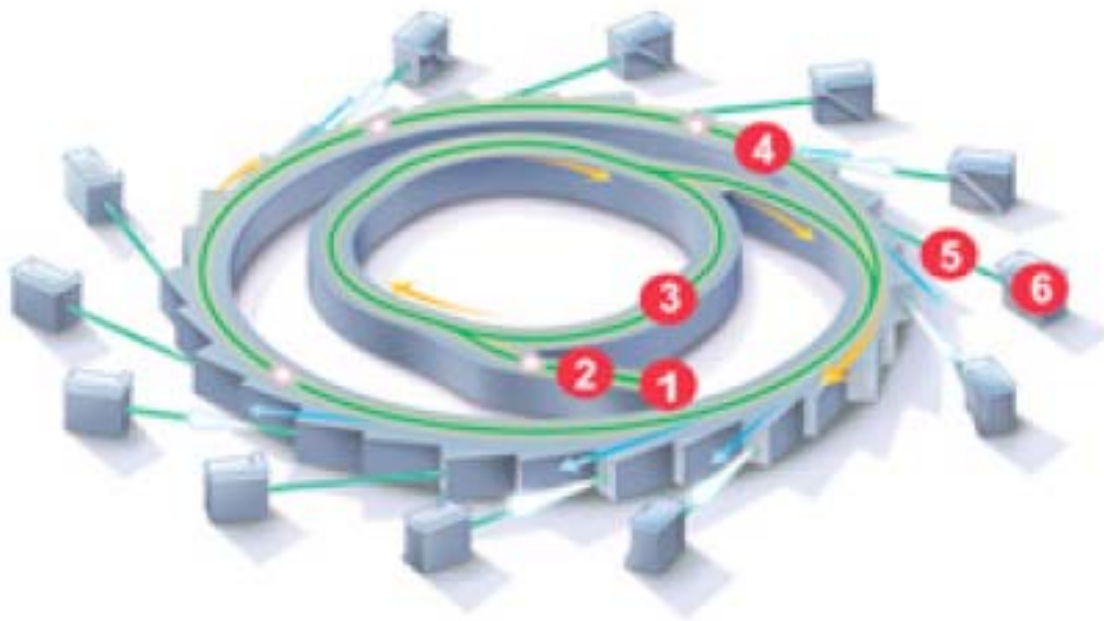
- High throughput
- Time-resolution (ms)
- Tunable energy (ASAXS)
- Micro & nanofocused beams for scanning (diffraction, imaging)
- Ultrathin films (GISAXS)

- **Neutrons**

- Sensitive to light atoms: polymers, biology, soft condensed matter, hydrogen in metals
- Isotope labeling (Multi-component systems)
- No radiation damage
- High penetration
 - bulky specimens
 - complicated environments (P,T)
- Magnetic contrast

Neutron scattering length

How do we produce X-rays?



1. Electron gun
2. Linear Accelerator LINAC
3. Booster Synchrotron
4. Storage Ring (SR)
5. Beamline
6. Experiment station

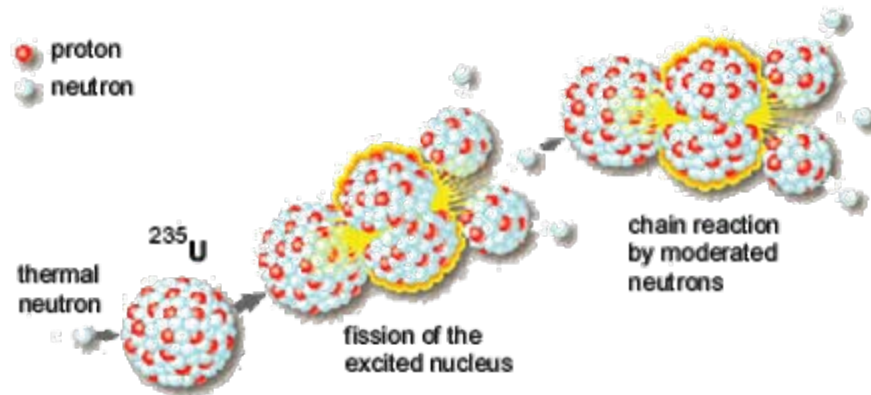
(Courtesy: Australian Synchrotron,
Illustrator: Michael Payne)

Argonne APS Facility

The Advanced Photon Source Accelerator Complex

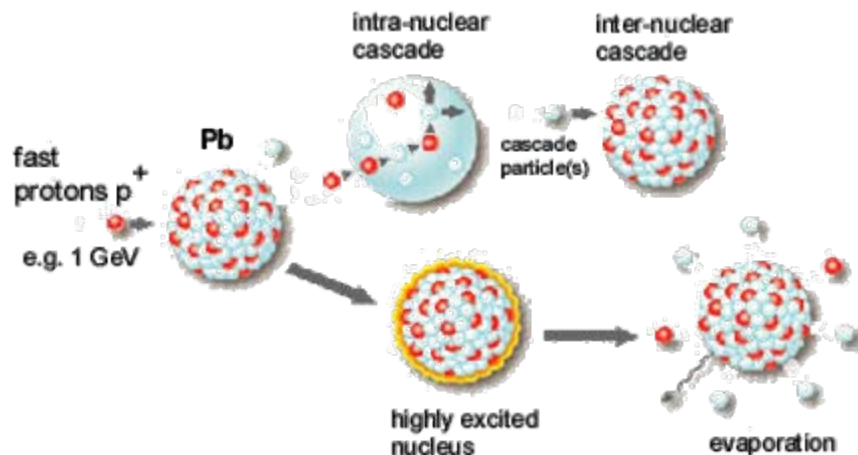


How do we produce neutrons?



Fission

- Chain reaction
- Continuous flow
- ~ 1 neutron/fission



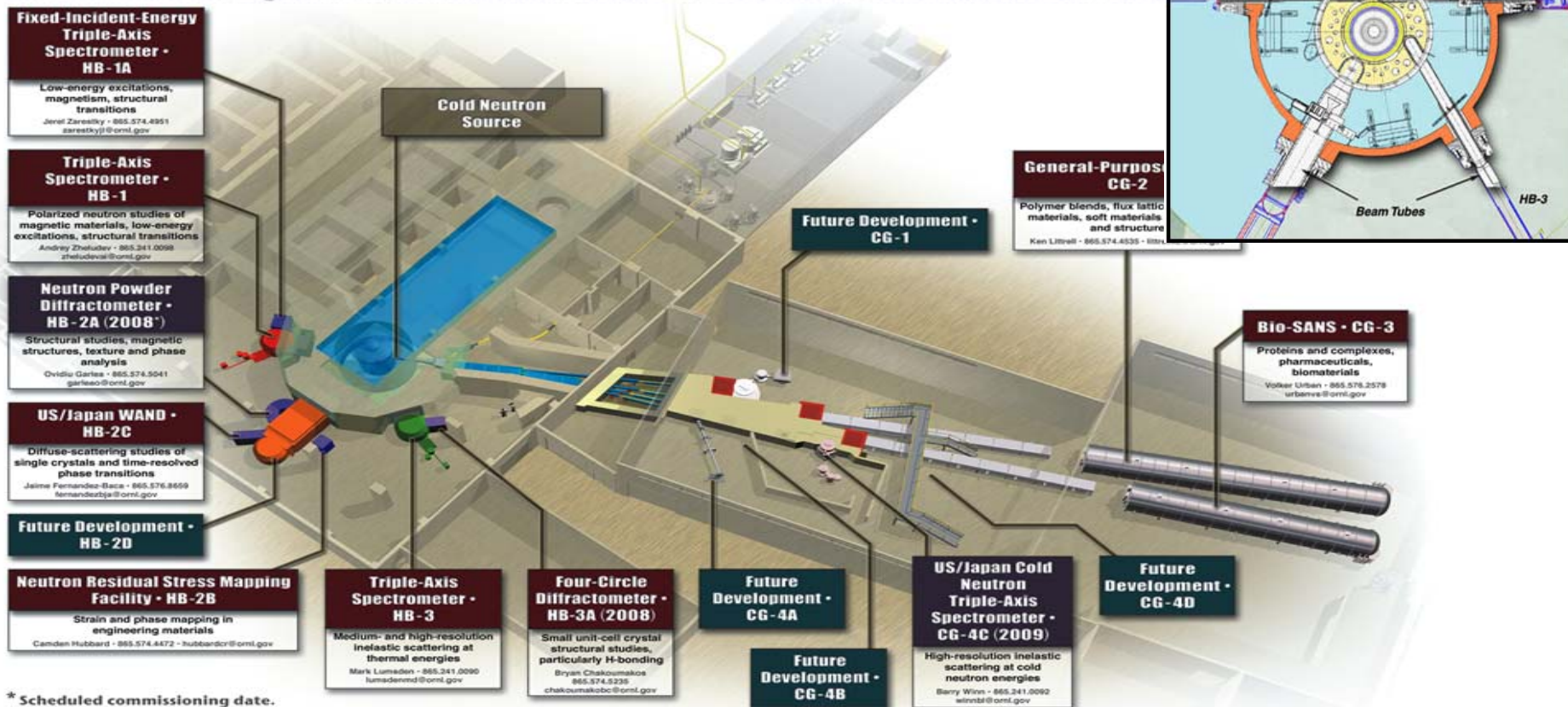
Spallation

- No chain reaction
- Accelerator driven
- Pulsed operation
- ~ 30 neutrons/proton

Oak Ridge Facility ----HFIR

The HFIR is a beryllium-reflected, light-water-cooled and -moderated, flux-trap type reactor that uses highly enriched uranium-235 as the fuel.

High Flux Isotope Reactor at Oak Ridge National Laboratory The United States' highest flux reactor-based source of neutrons for condensed matter research



* Scheduled commissioning date.

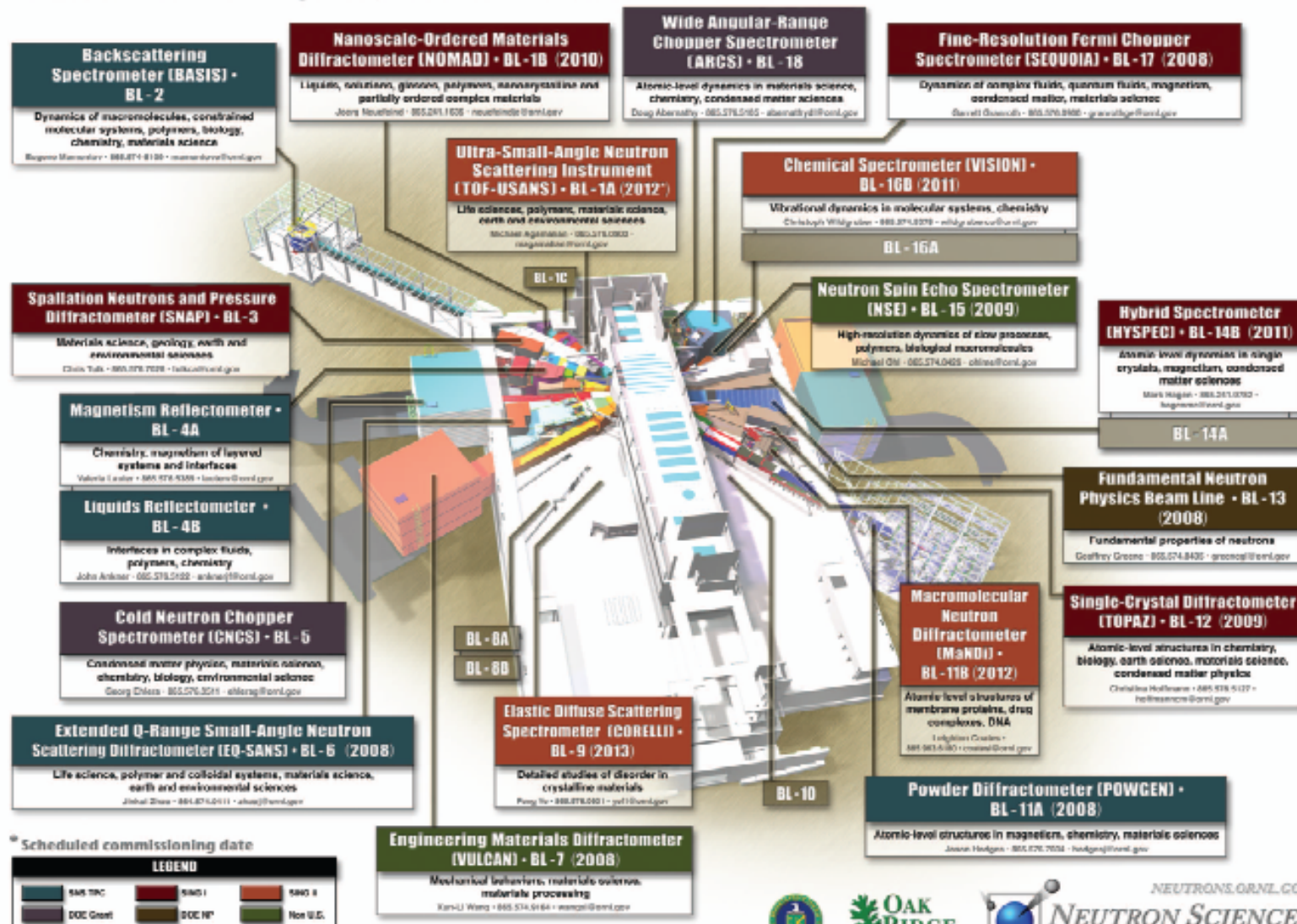
LEGEND	
	Installed, commissioning, or operating
	In design or construction
	Under consideration

Oak Ridge Facility--SNS

Spallation Neutron Source at Oak Ridge National Laboratory



The world's most intense pulsed, accelerator-based neutron source



Experiments

Neutron:

- Triple Axis Spectrometer
- Small Angle Neutron Scattering(SANS)
- Wide Angular-Range Chopper Spectrometer (ARCS)

X-Ray:

- Small Angle X-ray Scattering(SAXS)
- High Pressure Powder Diffraction
- X-ray Computed Micro-Tomography(XCMT)

Triple-axis Spectrometer

The Nobel Prize in Physics 1994



Clifford G. Shull, MIT, Cambridge, Massachusetts, USA, winner one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.



S Shull made use of elastic scattering, i.e. of neutrons which change direction without losing energy, when they collide with atoms.

Because of the wave nature of neutrons, a diffraction pattern can be recorded which indicates where in the sample the atoms are situated. From the placing of light elements, such as hydrogen, carbon or oxygen in organic substances can be determined.

The pattern also shows how atoms, dipoles are oriented in magnetic materials, since neutrons are affected by magnetic forces. Shull also made use of this phenomenon in his neutron diffraction technique.



Shull working in his laboratory. Photo courtesy of the American Museum of Natural History.

Neutrons show where atoms are

When the neutrons collide with atoms in the sample material, they change direction and sometimes lose energy.

Neutrons bounce against atomic nuclei. They also react to the magnetism of the atoms.

Neutrons record the direction of the neutrons and a diffraction pattern is obtained. The pattern shows the positions of the atoms in the sample.

Crystal that scatters and forwards neutrons of a certain wavelength energy - elastic scattering

Neutrons show what atoms do

When the neutrons penetrate the sample they start to vibrate in the atoms. If the neutrons vibrate in phase or out of phase, the neutrons can be energy from atoms - inelastic scattering

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Neutrons behave as particles and as waves

The Royal Swedish Academy of Sciences has awarded the 1994 Nobel Prize in Physics for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter.

Bruno N. Brockhouse, McGill University, Montreal, Canada, winner one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.



B Brockhouse made use of inelastic scattering, i.e. of neutrons, which change both direction and energy when they collide with atoms. They then start to record atomic vibrations in crystals and record resonances in liquids and solids. Neutrons can also interact with gas atoms in magnets.

With his 3-axis spectrometer Brockhouse measured energies of phonons (atomic vibrations) and magnons (magnetic waves). He also studied how atomic structure in liquids change with time.

When the neutrons penetrate the sample they start to vibrate in the atoms. If the neutrons vibrate in phase or out of phase, the neutrons can be energy from atoms - inelastic scattering

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Neutrons see more than X-rays

X-rays are scattered by electrons, located in atoms nuclei. With X-rays, only the positions of the atoms can be determined. Neutrons, on the other hand, are scattered by the nuclei of the atoms. This means that neutrons can see the positions of the atoms in the sample.



Neutrons reveal inner stresses

Neutrons can be used to study the internal stresses in materials. This is done by measuring the change in the neutron wavelength when it is scattered by the atoms in the material. The change in wavelength is proportional to the internal stress.



Neutrons show what atoms remember

Neutrons can be used to study the memory of atoms. This is done by measuring the change in the neutron wavelength when it is scattered by the atoms in the material. The change in wavelength is proportional to the memory of the atoms.



How it started

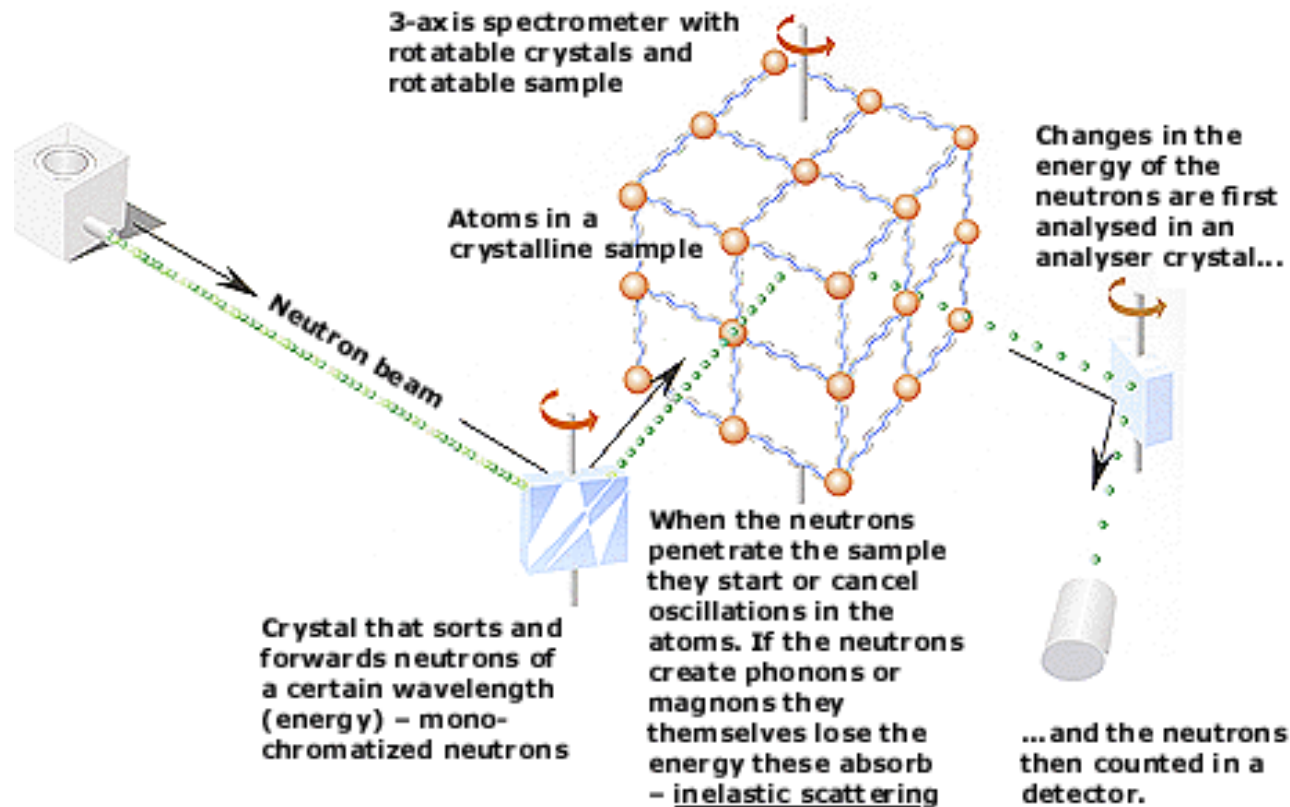
Brockhouse and Shull made their pioneering contributions to the field of neutron scattering in the USA and Canada. They were the first to use neutrons for the study of condensed matter.

How it continues

Thousands of scientists around the world now use neutron scattering to study the structure and dynamics of condensed matter. This is done by measuring the change in the neutron wavelength when it is scattered by the atoms in the material. The change in wavelength is proportional to the structure and dynamics of the material.



KUNGLIGA VETENSKAPSAKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES



Momentum transfer

$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

Energy transfer

$$E = \hbar\omega = \hbar k_i^2/2m - \hbar k_f^2/2m$$

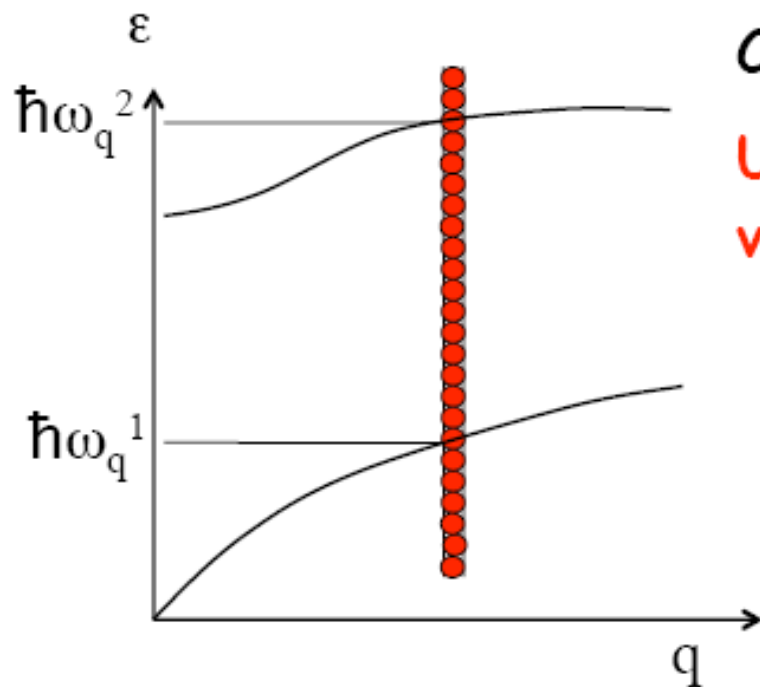
Inelastic scattering

$\hbar\omega > 0$ "Energy loss"

$\hbar\omega < 0$ "Energy gain"



Constant Q and Constant ϵ Scans

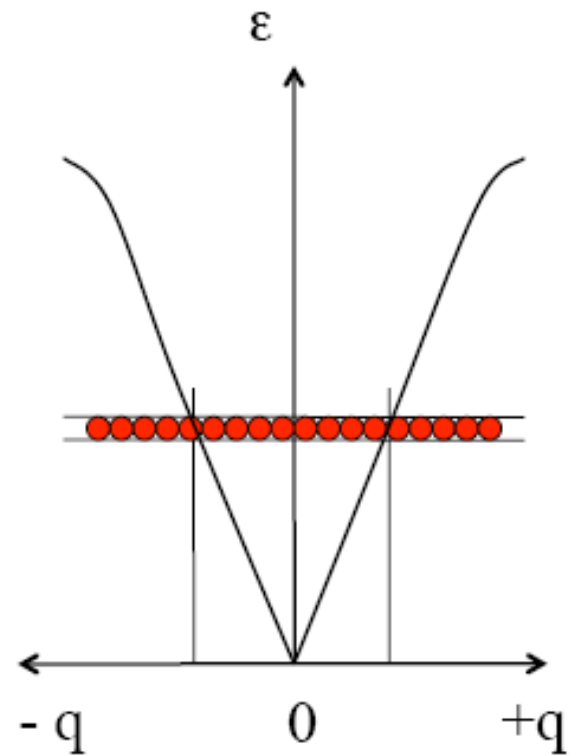


Constant Q scan

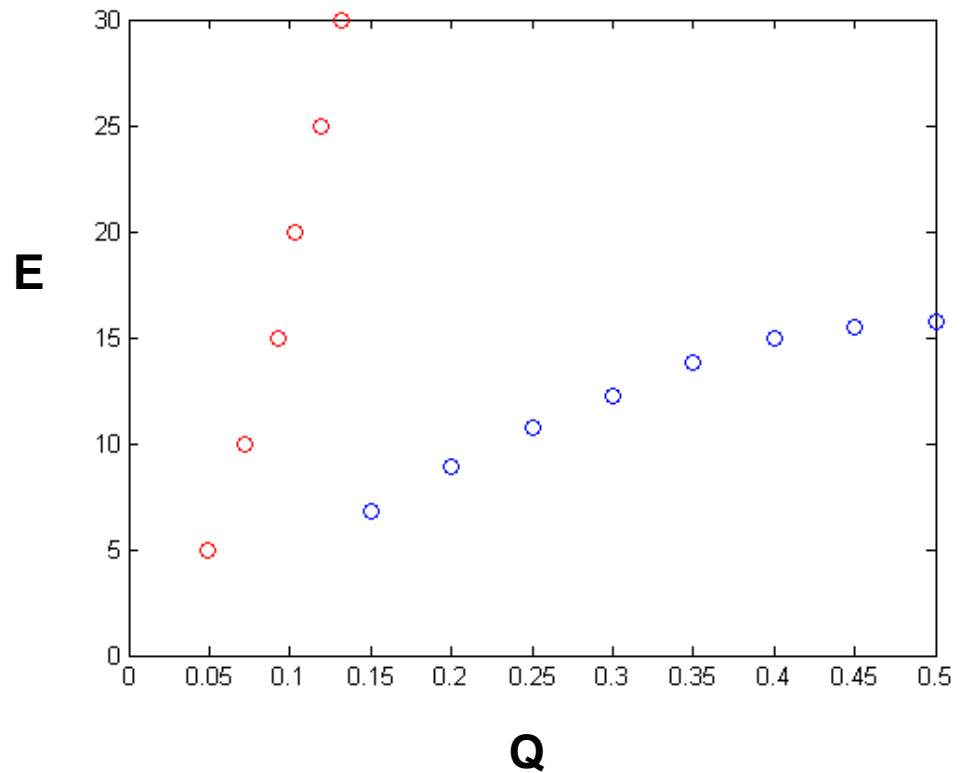
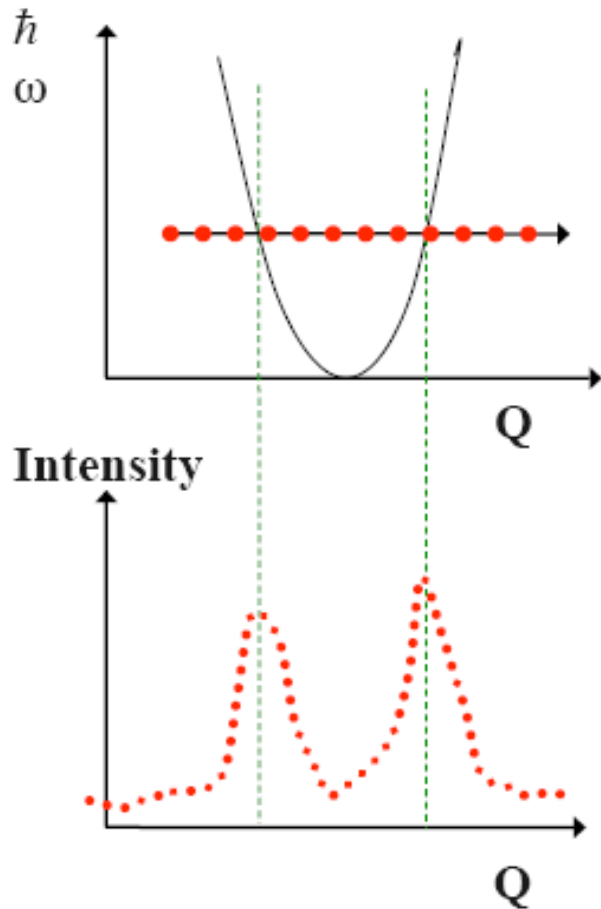
Used to measure slowly
varying dispersion relations.

Constant ϵ scan

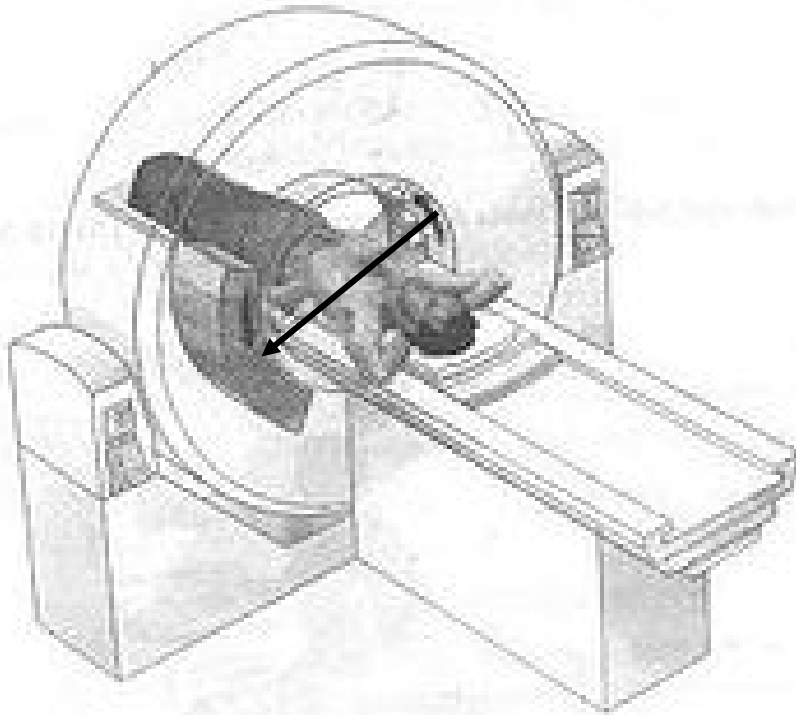
Used to measure steep
Dispersion relations.



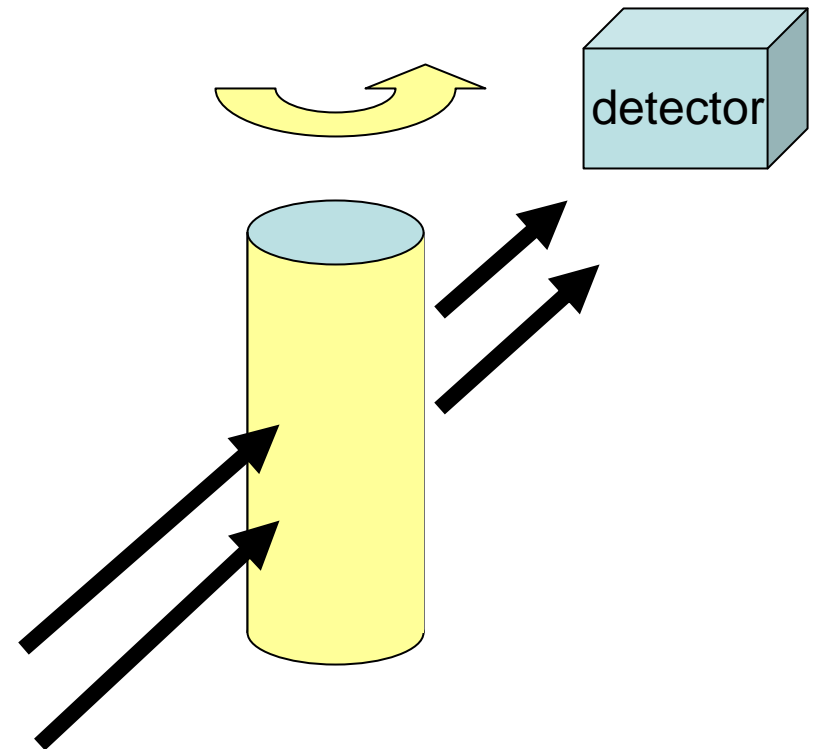
Dispersion Relation of Fe-Ga Alloy



Computed X-ray Micro-Tomography ----CMT

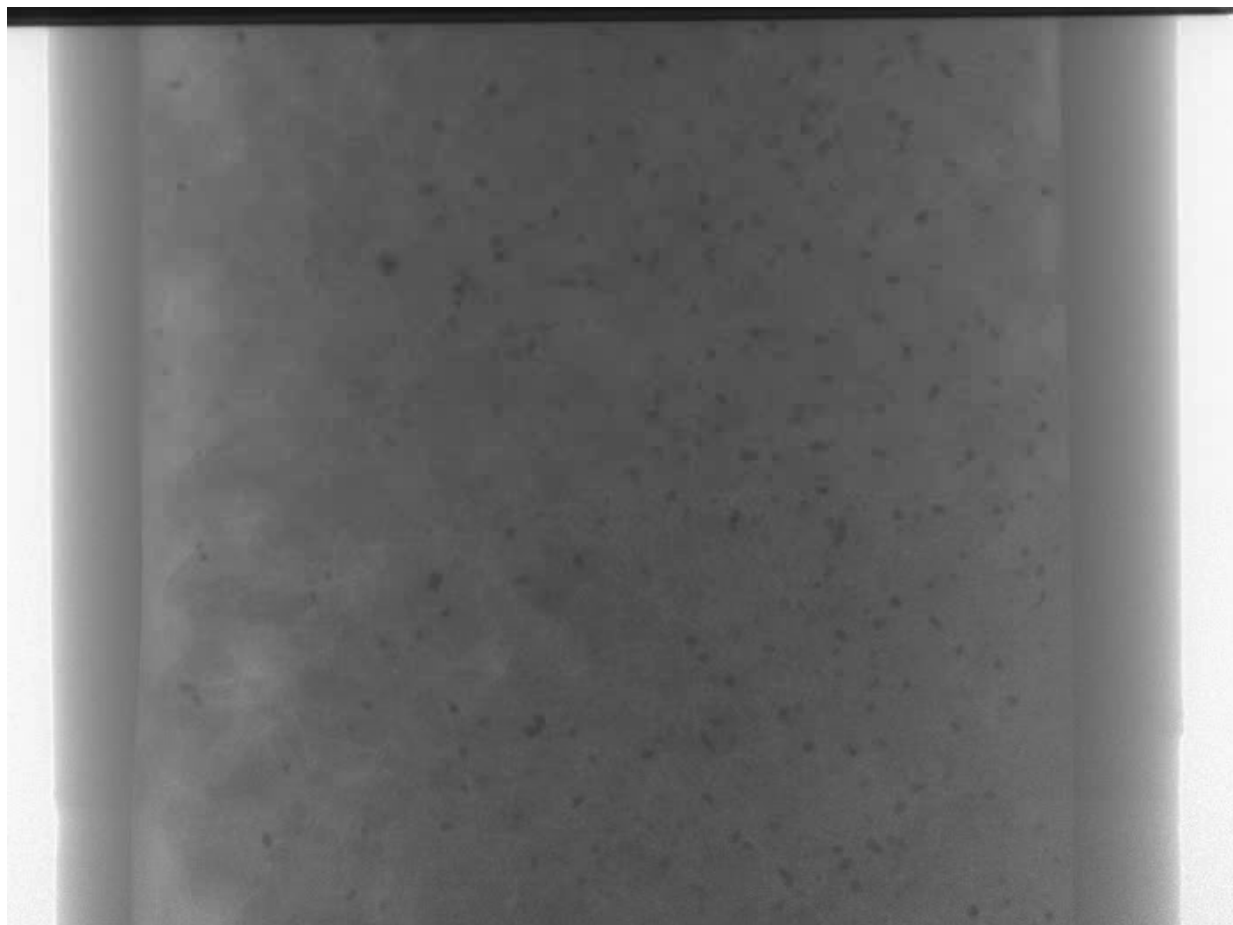
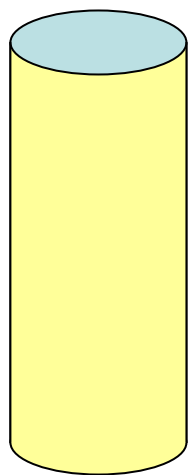


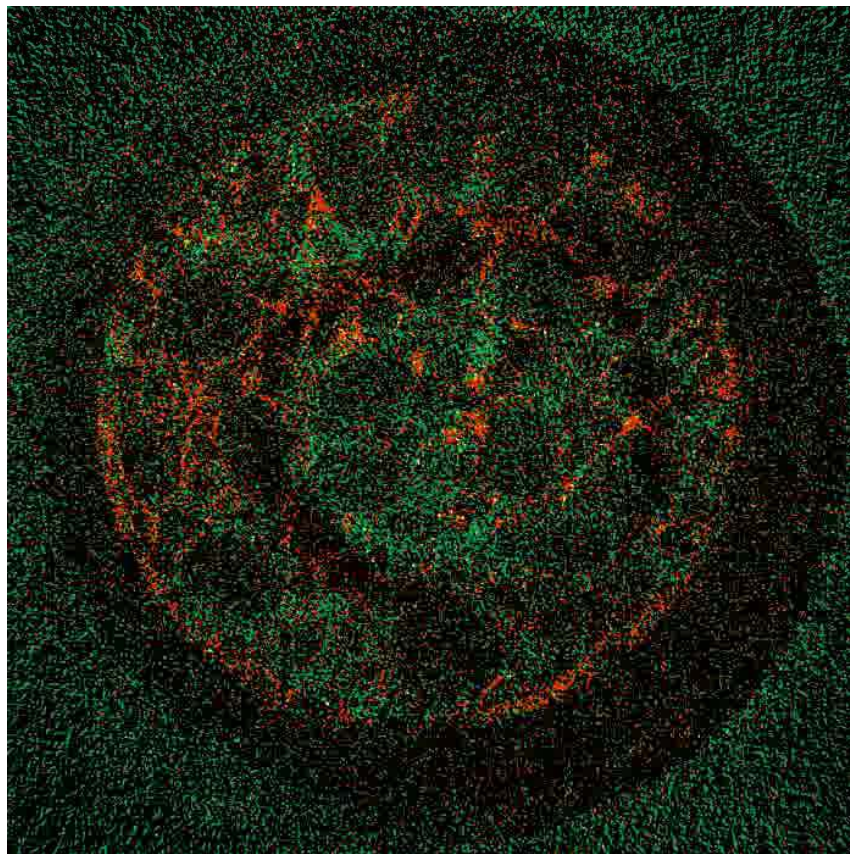
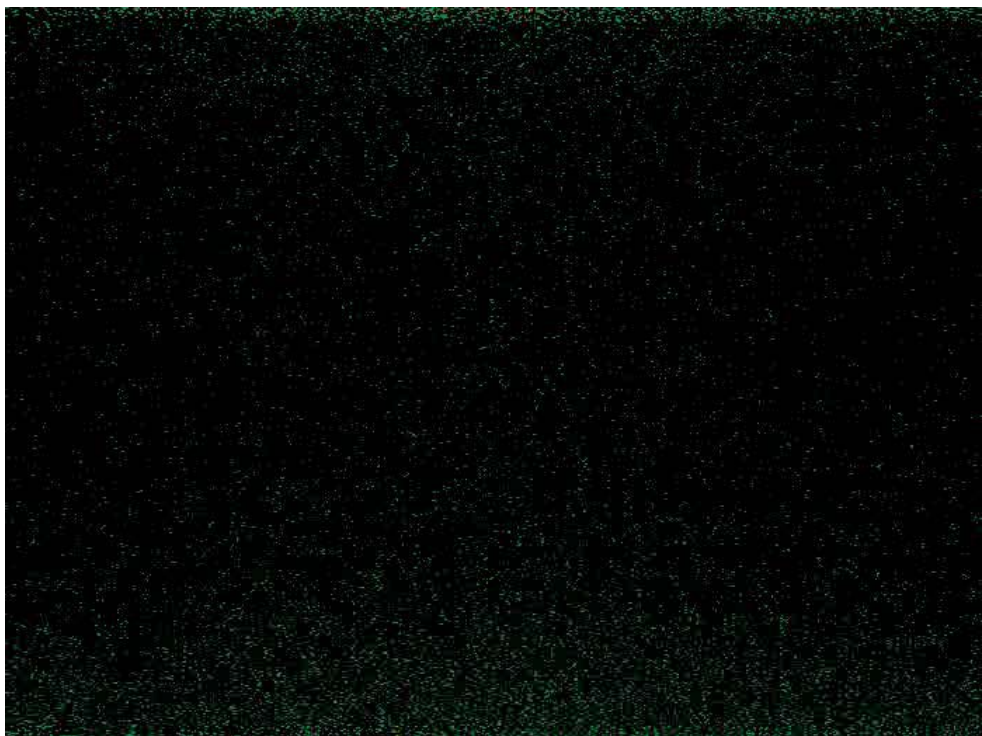
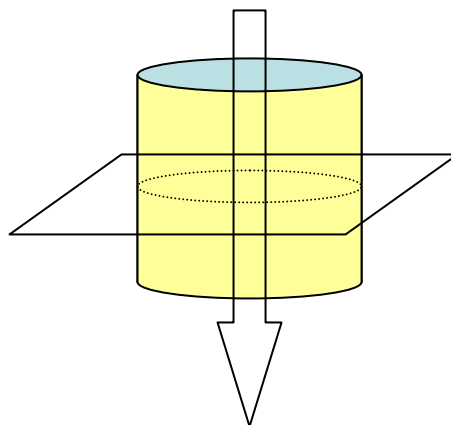
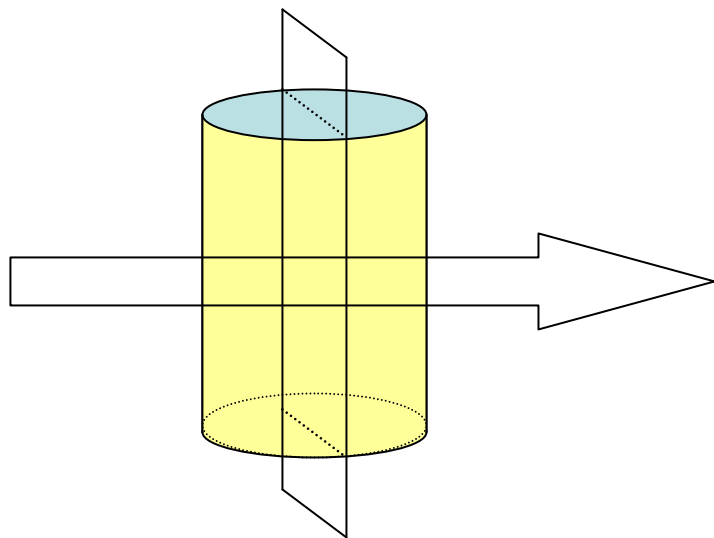
Medical Imaging CT
0.5-1mm resolution



Micro-CT
Down to 1 micro

- Sample: a soil that contains water, solid and oil
 - Goal: to image the distribution of two liquids in soil
 - Contrast: enhance the contrast by doping water with cesium(Cs) and doping the oil with iodine (I).
 - Energies: 100eV above and below the I K absorption edge (33.139 keV) and 100eV above and below the Cs K absorption edge (36.985keV)
 - measuring the transmitted x-ray image as the sample is rotated 180 degrees in 0.25 degree steps
-
- data → normalization → reconstruction(FFT tech)
→ 3-D cross-sections





Thank you!

The Advanced Photon Source Accelerator Complex

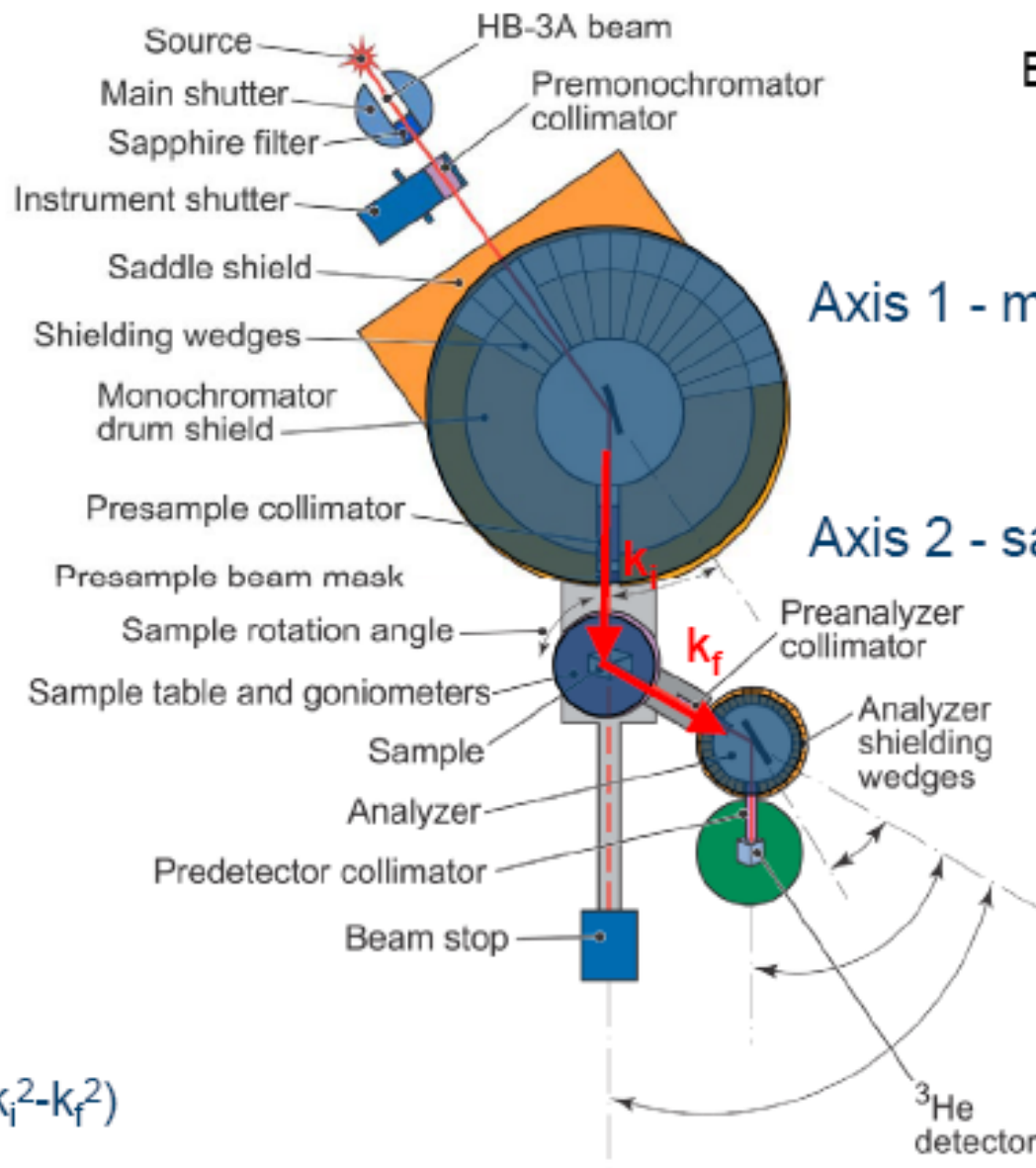


NXschool Lectures

- **Interaction of X-rays and Neutrons with Matter** -- D. F. McMorrow
- **Real/Reciprocal Space/Complementarity** -- J. M. Gibson
- **Powder Diffraction** -- J. J. Rhyne
- **Reflectivity/Magnetic Scattering** -- C. F. Majkrzak
- **Single Crystal Diffraction** -- X. Wang
- **Diffuse Scattering/Micro-Diffraction** -- G. E. Ice
- **Powder Diffraction Applications** -- A. Huq
- **PDF Analysis** -- T. E. Proffen
- **Small Angle Scattering** -- S. Krueger
- **High-Pressure Techniques** -- W. Mao
- **Magnetic Spectroscopy and Scattering** -- E. Fullerton
- **Neutron and X-rays for NanoScience** -- E. D. Isaacs

- **X-ray Generation/Instrumentation** -- D. M. Mills
- **X-ray Detection/Sources** -- S. M. Gruner
- **Synchrotron Sources** -- P. Zschack
- **X-ray Absorption Fine Structure (XAFS)** -- G. B. Bunker
- **Coherent X-ray Scattering** -- L. B. Lurio
- **Inelastic X-ray Scattering** -- P. M. Abbamonte
- **X-ray Imaging** -- S. R. Stock
- **Time-Resolved X-ray Scattering** -- D. A. Reis

- **Neutron Generation/Detection** -- J. M. Carpenter
- **Neutron Sources** -- J. J. Rhyne
- **Quasi-elastic Neutron Scattering** -- K. W. Herwig
- **Inelastic Neutron Scattering** -- R. Osborn
- **Spin-Echo Techniques** -- R. Pynn



Bragg's Law:
 $\lambda = 2d \sin \theta$

Axis 1 - monochromator

Axis 2 - sample

Axis 3 - analyzer



$$Q = k_i - k_f$$

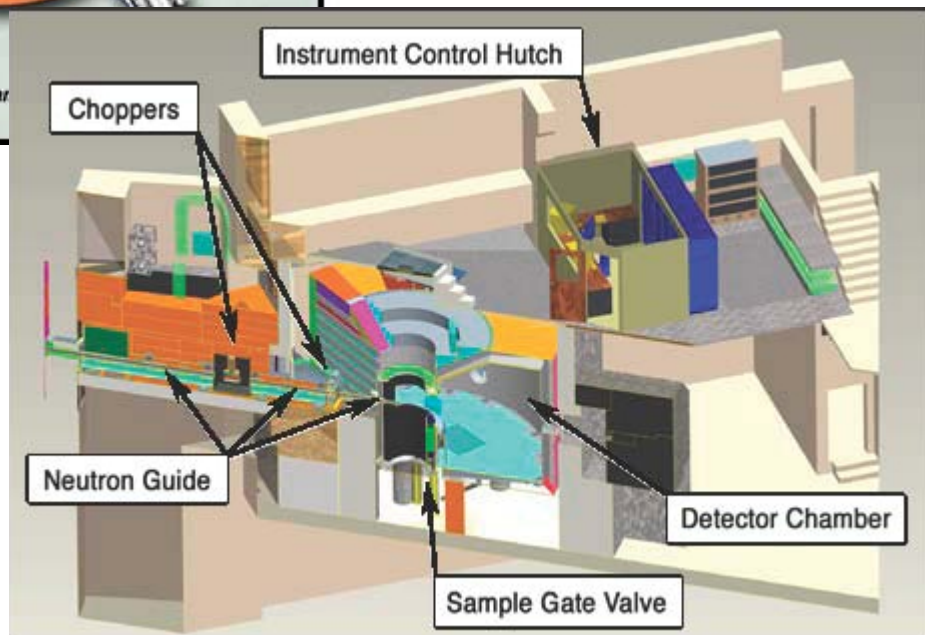
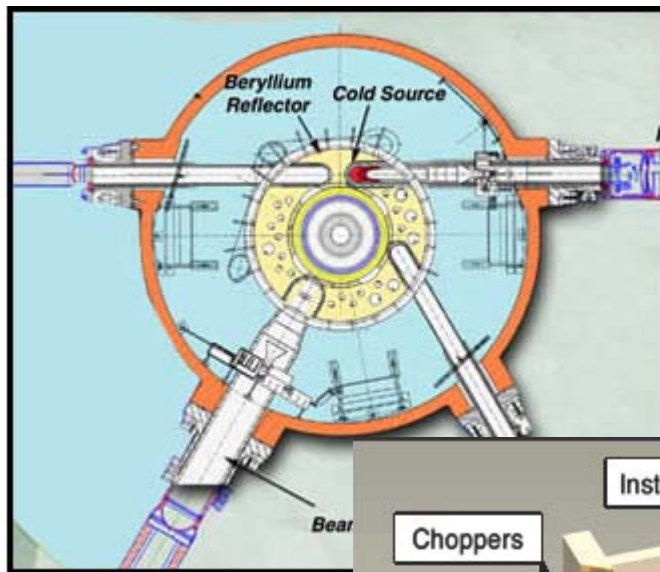
$$\Delta E = (\hbar^2/2m)(k_i^2 - k_f^2)$$

Inelastic scattering

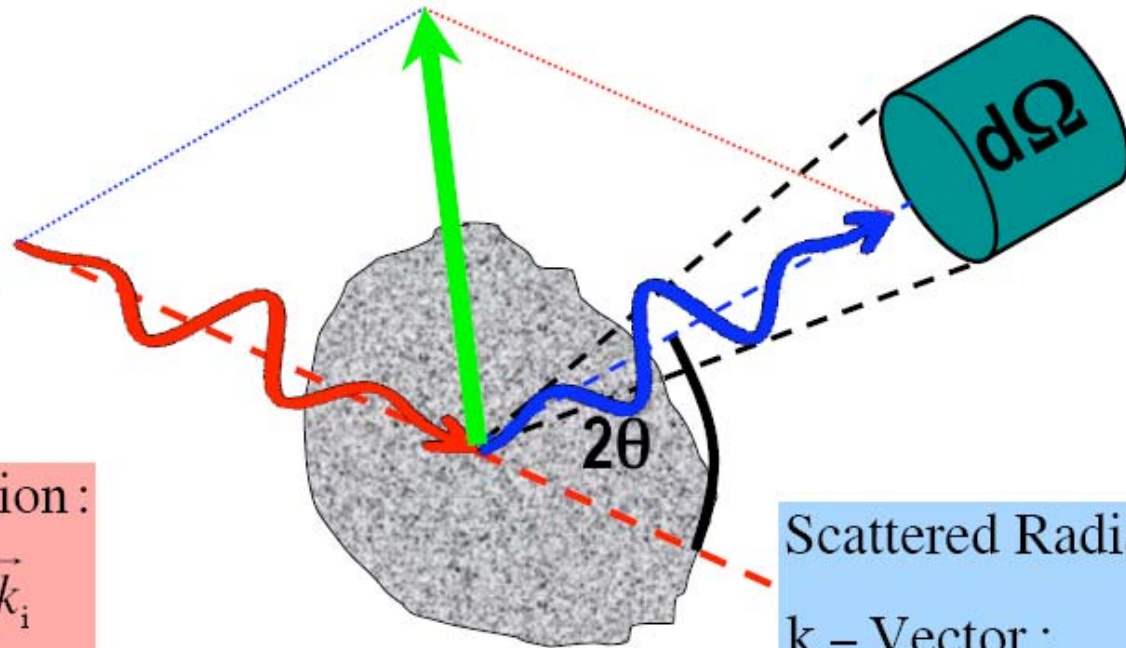
$\hbar\omega > 0$ "Energy loss"

$\hbar\omega < 0$ "Energy gain"





Scattering Geometry



Incident Radiation:

k - Vector: \vec{k}_i

$$|\vec{k}_i| = 2\pi / \lambda$$

Energy: E_i

Polarization: \vec{p}_i

Scattered Radiation:

k - Vector: \vec{k}_f

Energy: E_f

Polarization: \vec{p}_f

Wavevector Transfer:

$$\vec{q} = \vec{k}_f - \vec{k}_i$$

Energy Transfer:

$$\Delta E = E_f - E_i = \hbar \omega$$

Polarization:

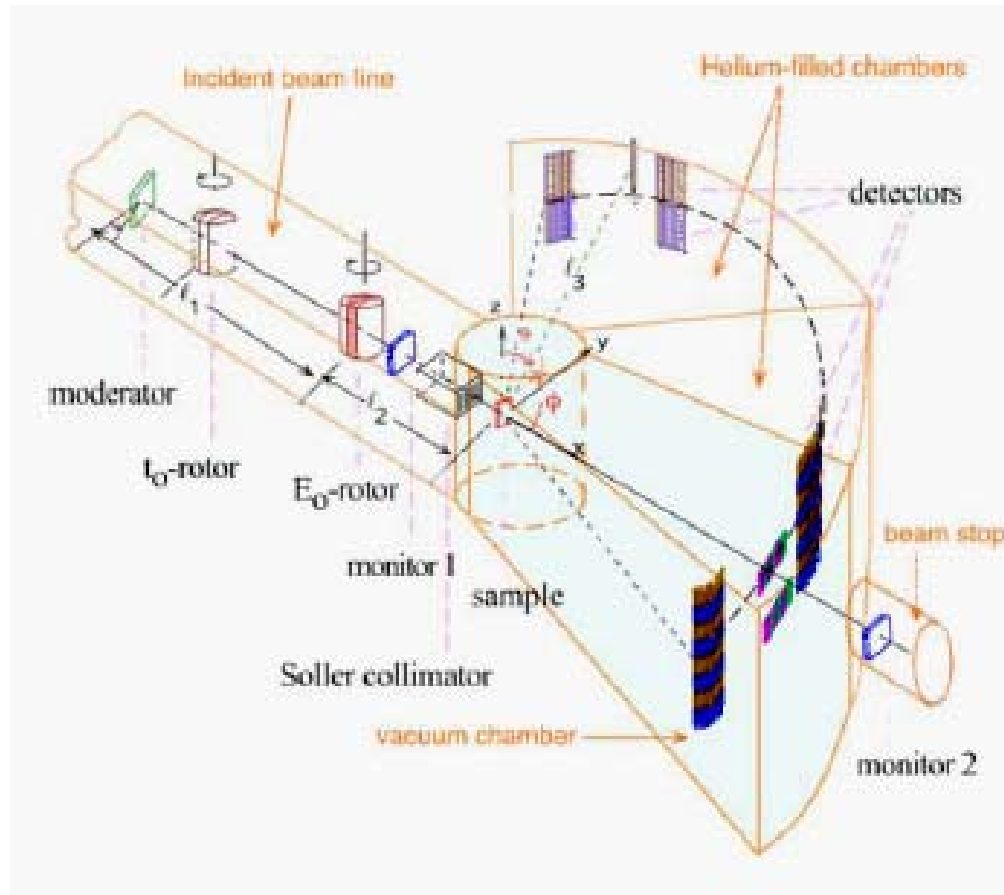
$$\vec{p}_i \rightarrow \vec{p}_f$$

For X - Rays:

$$\Delta E \ll E_f, E_i$$

$$\Rightarrow |\vec{q}| = 2k_i \sin(2\theta / 2)$$

Wide Angular-Range Chopper Spectrometer (ARCS)



- Primary Flight Path: 11.6m
- Secondary Flight Path: 3m
- Angular range :
 - 30° - 150° (Horizontal)
 - 30° - 30° (Vertical)
- Incident energy : 10meV-1.5eV
- Energy resolution : 2-5% E_i
- Detectors : Position sensitive
- Supermirror guide
- Oscillating collimator
- Provision for polarization analysis

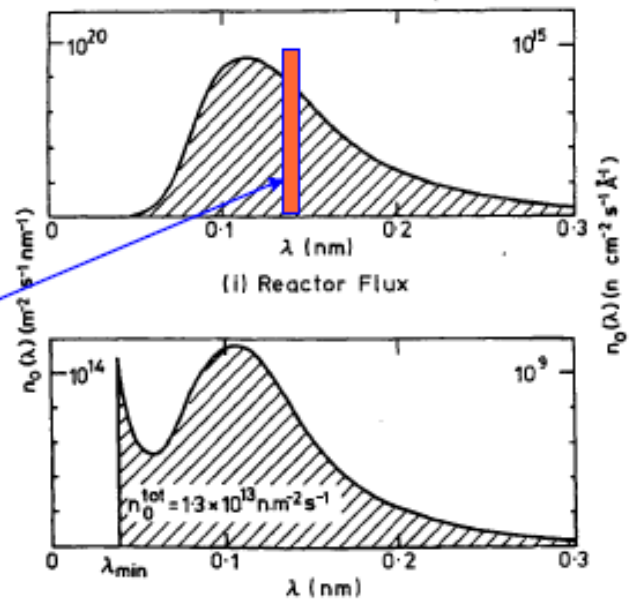
X-rays, Neutrons and Electrons

	X-rays	Neutrons	Electrons
	$\lambda = \frac{hc}{E}$	$\lambda = \frac{h}{\sqrt{2m_n E}}$	$\lambda = \frac{h}{\sqrt{2m_e E}}$
Practical Units	$\lambda[\text{\AA}] = \frac{12.4}{E[\text{keV}]}$	$\lambda[\text{\AA}] = \frac{9.08}{\sqrt{E[\text{meV}]}}$	$\lambda[\text{\AA}] = \frac{12.3}{\sqrt{E[\text{eV}]}}$
Energy Range	1-100 keV	10-1000 meV	10-10 ⁵ eV
Wavelength Range [Å]	10-0.1	3-0.3	4-0.04
Penetration Depth	1-100 μm	1-50 mm	1-100 Å

Neutron sources – steady state (Reactors) and pulsed (Spallation)

◆ Reactor

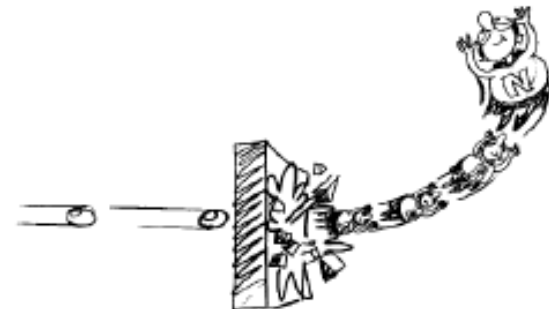
- Fission of U^{235} produces neutrons
- Fission spectrum moderated (slowed down) by either D_2O or H_2O (less good moderator) and neutrons are extracted through beam tubes for spectrometers – fixed wavelength used



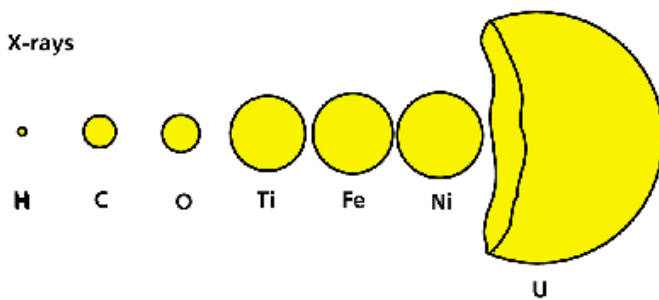
◆ Spallation source

- High E protons (e.g., 800 MeV) impinge on target (W, Hg or U)
- Nucleus of target is raised to excited state and subsequent decay produces neutrons (+ γ s, nucleons and neutrinos) – 15 – 25 neutrons produced per proton with average $E = 55 \text{ MeV}$
- Neutrons moderated by liquid H, H_2O or methane
- Spallation sources generally operate in pulse mode – 20 Hz at LANSCE, 60 Hz at new SNS

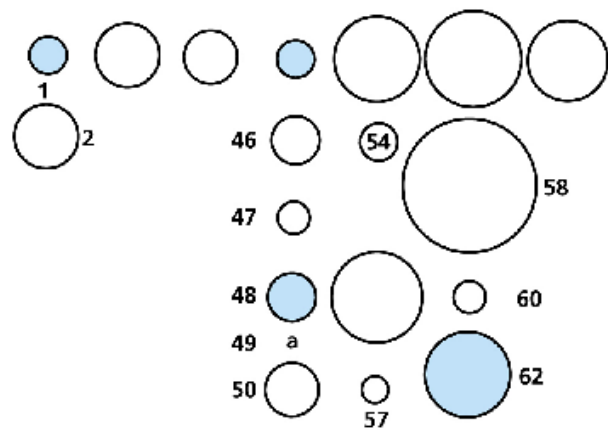
Time of flight is used to sort out wavelengths



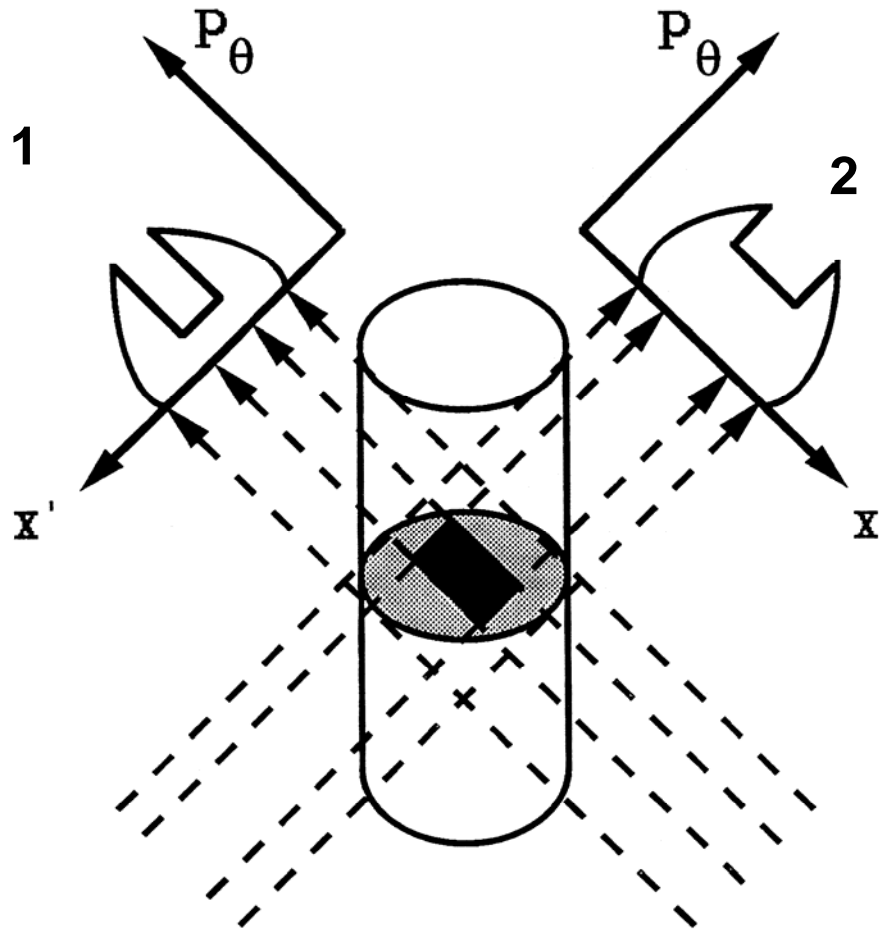
X-rays



Neutrons



How reconstruction works (cartoon)



Along direction 1, the high absorption rectangle makes a spatially narrow but deep “valley” in the absorption profile P_θ .

Along direction 2, the profile P_θ has a spatially wide, but shallow “valley”.

At intermediate angles the edges of the valley are less sharp.